Michael Nilges

List of Publications by Year in Descending Order

220 papers	29,429 citations	65 h-index	171 g-index
247 ext. papers	30,893 ext. citations	6.9 avg, IF	6.47 L-index

#	Paper	IF	Citations
220	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells.. *Nature*, **2022**,	50.4	36
219	quicksom: Self-Organizing Maps on GPUs for clustering of molecular dynamics trajectories. *Bioinformatics*, **2021**, 37, 2064-2065	7.2	4
218	Automatic Bayesian Weighting for SAXS Data. *Frontiers in Molecular Biosciences*, **2021**, 8, 671011	5.6	1
217	Host-Pathogen Adhesion as the Basis of Innovative Diagnostics for Emerging Pathogens. *Diagnostics*, **2021**, 11,	3.8	3
216	The iPPI-DB initiative: A Community-centered database of Protein-Protein Interaction modulators. *Bioinformatics*, **2021**,	7.2	4
215	Structural determination of Streptococcus pyogenes M1 protein interactions with human immunoglobulin G using integrative structural biology. *PLoS Computational Biology*, **2021**, 17, e1008169	5	3
214	H, N and C resonance assignments of the C-terminal domain of PulL, a component of the Klebsiella oxytoca type II secretion system. *Biomolecular NMR Assignments*, **2021**, 15, 455-459	0.7	0
213	Computational and biochemical analysis of type IV pilus dynamics and stability. *Structure*, **2021**, 29, 1397-1409.e6	5.2	1
212	InDeep: 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions.. *Bioinformatics*, **2021**,	7.2	2
211	Bayesian inference of chromatin structure ensembles from population-averaged contact data. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 7824-7830	11.5	5
210	Quantitative Structural Interpretation of Protein Crosslinks. *Structure*, **2020**, 28, 75-82.e4	5.2	4
209	Structure and function of minor pilins of type IV pili. *Medical Microbiology and Immunology*, **2020**, 209, 301-308	4	20
208	ARIAweb: a server for automated NMR structure calculation. *Nucleic Acids Research*, **2020**, 48, W41-W47	20.1	3
207	Dynamics of a type 2 secretion system pseudopilus unraveled by complementary approaches. *Journal of Biomolecular NMR*, **2019**, 73, 293-303	3	6
206	Structure and Assembly of the Enterohemorrhagic Escherichia coli Type 4 Pilus. *Structure*, **2019**, 27, 1082-1093.e5	5.2	23
205	: Consistent Identification of Plausible Binding Sites Despite the Elusive Nature of Cavities and Grooves in Protein Dynamics. *Journal of Chemical Information and Modeling*, **2019**, 59, 3506-3518	6.1	9
204	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. *Structure*, **2019**, 27, 175-188.e6	5.2	24

203	Target Engagement and Binding Mode of an Antituberculosis Drug to Its Bacterial Target Deciphered in Whole Living Cells by NMR. *Biochemistry*, **2019**, 58, 526-533	3.2	11
202	Minimal NMR distance information for rigidity of protein graphs. *Discrete Applied Mathematics*, **2019**, 256, 91-104	1	19
201	Sequence-specific DNA binding activity of the cross-brace zinc finger motif of the piggyBac transposase. *Nucleic Acids Research*, **2018**, 46, 2660-2677	20.1	14
200	Ordering Protein Contact Matrices. *Computational and Structural Biotechnology Journal*, **2018**, 16, 140-156	3.8	8
199	Tuning interval Branch-and-Prune for protein structure determination. *Journal of Global Optimization*, **2018**, 72, 109-127	1.5	12
198	Identification of novel leishmanicidal molecules by virtual and biochemical screenings targeting Leishmania eukaryotic translation initiation factor 4A. *PLoS Neglected Tropical Diseases*, **2018**, 12, e0006160	4.8	13
197	Automatic Building of Protein Atomic Models from Cryo-EM Maps. *Biophysical Journal*, **2018**, 114, 190a-191a	2.9	2
196	Conformational sampling of CpxA: Connecting HAMP motions to the histidine kinase function. *PLoS ONE*, **2018**, 13, e0207899	3.7	1
195	Nicotine reverses hypofrontality in animal models of addiction and schizophrenia. *Nature Medicine*, **2017**, 23, 347-354	50.5	107
194	Structural Characterization of Whirlin Reveals an Unexpected and Dynamic Supramodule Conformation of Its PDZ Tandem. *Structure*, **2017**, 25, 1645-1656.e5	5.2	16
193	Structure of the calcium-dependent type 2 secretion pseudopilus. *Nature Microbiology*, **2017**, 2, 1686-1695	25.6	38
192	In Silico prediction of the molecular basis of ClTx and AaCTx interaction with matrix metalloproteinase-2 (MMP-2) to inhibit glioma cell invasion. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2815-2829	3.6	12
191	SAS profile correlations reveal SAS hierarchical nature and information content. *PLoS ONE*, **2017**, 12, e0177309	3.7	5
190	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. *Bioinformatics*, **2016**, 32, 85-95	7.2	60
189	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling. *Molecular and Cellular Proteomics*, **2016**, 15, 2730-43	7.6	46
188	Inferential Structure Determination of Chromosomes from Single-Cell Hi-C Data. *PLoS Computational Biology*, **2016**, 12, e1005292	5	36
187	Modification in hydrophobic packing of HAMP domain induces a destabilization of the auto-phosphorylation site in the histidine kinase CpxA. *Biopolymers*, **2016**, 105, 670-82	2.2	2
186	Automated structure modeling of large protein assemblies using crosslinks as distance restraints. *Nature Methods*, **2016**, 13, 515-20	21.6	44

185	Building Graphs To Describe Dynamics, Kinetics, and Energetics in the d-ALa:d-Lac Ligase VanA. *Journal of Chemical Information and Modeling*, **2016**, 56, 1762-75	6.1	4
184	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. *Journal of Chemical Theory and Computation*, **2015**, 11, 3446-54	6.4	11
183	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67	5.2	131
182	Improved reliability, accuracy and quality in automated NMR structure calculation with ARIA. *Journal of Biomolecular NMR*, **2015**, 62, 425-38	3	18
181	An algorithm to enumerate all possible protein conformations verifying a set of distance constraints. *BMC Bioinformatics*, **2015**, 16, 23	3.6	32
180	Identification of binding sites and favorable ligand binding moieties by virtual screening and self-organizing map analysis. *BMC Bioinformatics*, **2015**, 16, 93	3.6	11
179	Principal Component Analysis reveals correlation of cavities evolution and functional motions in proteins. *Journal of Molecular Graphics and Modelling*, **2015**, 55, 13-24	2.8	29
178	SAS Profile Correlations Reveal the Hierarchical Nature of SAS Data and Suggest New Scoring Strategies. *Biophysical Journal*, **2015**, 108, 45a	2.9	
177	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nature Structural and Molecular Biology*, **2015**, 22, 433-4	17.6	26
176	An automatic tool to analyze and cluster macromolecular conformations based on self-organizing maps. *Bioinformatics*, **2015**, 31, 1490-2	7.2	19
175	Neisseria meningitidis Type IV Pili Composed of Sequence Invariable Pilins Are Masked by Multisite Glycosylation. *PLoS Pathogens*, **2015**, 11, e1005162	7.6	42
174	Functional motions modulating VanA ligand binding unraveled by self-organizing maps. *Journal of Chemical Information and Modeling*, **2014**, 54, 289-301	6.1	11
173	Convective Replica-Exchange in Ergodic Regimes. *Journal of Chemical Theory and Computation*, **2014**, 10, 953-8	6.4	3
172	Computational design of protein-based inhibitors of Plasmodium vivax subtilisin-like 1 protease. *PLoS ONE*, **2014**, 9, e109269	3.7	1
171	ModBase, a database of annotated comparative protein structure models and associated resources. *Nucleic Acids Research*, **2014**, 42, D336-46	20.1	207
170	Stabilization of the integrase-DNA complex by Mg2+ ions and prediction of key residues for binding HIV-1 integrase inhibitors. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 466-78	4.2	12
169	Distinct docking and stabilization steps of the Pseudopilus conformational transition path suggest rotational assembly of type IV pilus-like fibers. *Structure*, **2014**, 22, 685-96	5.2	40
168	SAXS Merge: an automated statistical method to merge SAXS profiles using Gaussian processes. *Journal of Synchrotron Radiation*, **2014**, 21, 203-8	2.4	12

167	Recommendations of the wwPDB NMR Validation Task Force. *Structure*, **2013**, 21, 1563-70	5.2	117
166	In Silico screening on the three-dimensional model of the Plasmodium vivax SUB1 protease leads to the validation of a novel anti-parasite compound. *Journal of Biological Chemistry*, **2013**, 288, 18561-73	5.4	15
165	A convective replica-exchange method for sampling new energy basins. *Journal of Computational Chemistry*, **2013**, 34, 132-40	3.5	16
164	Distance Geometry in Structural Biology: New Perspectives **2013**, 329-350		10
163	Blind testing of routine, fully automated determination of protein structures from NMR data. *Structure*, **2012**, 20, 227-36	5.2	64
162	Efficient Modeling of Symmetric Protein Aggregates from NMR Data. *Angewandte Chemie*, **2012**, 124, 7022-7025	3.6	
161	Efficient modeling of symmetric protein aggregates from NMR data. *Angewandte Chemie - International Edition*, **2012**, 51, 6916-9	16.4	7
160	Computational approaches to the interpretation of NMR data for studying protein dynamics. *Chemical Physics*, **2012**, 396, 124-134	2.3	8
159	Lobeline Docking on AChBP and Nicotinic Receptors: Discriminating Importance of the Pocket Geometry and of the Ligand Configuration. *Letters in Drug Design and Discovery*, **2012**, 9, 54-62	0.8	2
158	ARIA for solution and solid-state NMR. *Methods in Molecular Biology*, **2012**, 831, 453-83	1.4	38
157	Modeling pilus structures from sparse data. *Journal of Structural Biology*, **2011**, 173, 436-44	3.4	34
156	Posttranslational modification of pili upon cell contact triggers N. meningitidis dissemination. *Science*, **2011**, 331, 778-82	33.3	149
155	Computational reverse-engineering of a spider-venom derived peptide active against Plasmodium falciparum SUB1. *PLoS ONE*, **2011**, 6, e21812	3.7	26
154	A role for specific collagen motifs during wound healing and inflammatory response of fibroblasts in the teleost fish gilthead seabream. *Molecular Immunology*, **2011**, 48, 826-34	4.3	36
153	Discrimination of agonists versus antagonists of nicotinic ligands based on docking onto AChBP structures. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 100-9	2.8	15
152	The redundancy of NMR restraints can be used to accelerate the unfolding behavior of an SH3 domain during molecular dynamics simulations. *BMC Structural Biology*, **2011**, 11, 46	2.7	1
151	Bayesian estimation of NMR restraint potential and weight: a validation on a representative set of protein structures. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1525-37	4.2	20
150	Grid computing for improving conformational sampling in NMR structure calculation. *Bioinformatics* , **2011**, 27, 1713-4	7.2	2

149	Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems. *Lecture Notes in Computer Science*, **2011**, 206-217	0.9	10
148	Architecture of the RNA polymerase II-TFIIF complex revealed by cross-linking and mass spectrometry. *EMBO Journal*, **2010**, 29, 717-26	13	322
147	Visualization of macromolecular structures. *Nature Methods*, **2010**, 7, S42-55	21.6	107
146	Simultaneous use of solution, solid-state NMR and X-ray crystallography to study the conformational landscape of the Crh protein during oligomerization and crystallization. *Advances and Applications in Bioinformatics and Chemistry*, **2010**, 3, 25-38	1.5	
145	Structural insights into serine-rich fimbriae from Gram-positive bacteria. *Journal of Biological Chemistry*, **2010**, 285, 32446-57	5.4	43
144	Detailed structural and assembly model of the type II secretion pilus from sparse data. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 13081-6	11.5	54
143	Comparative evaluation of 3D virtual ligand screening methods: impact of the molecular alignment on enrichment. *Journal of Chemical Information and Modeling*, **2010**, 50, 992-1004	6.1	47
142	Protein Structure Calculation using Ambiguous Restraints **2010**,		3
141	An Efficient Protocol for NMR-Spectroscopy-Based Structure Determination of Protein Complexes in Solution. *Angewandte Chemie*, **2010**, 122, 2011-2014	3.6	5
140	An efficient protocol for NMR-spectroscopy-based structure determination of protein complexes in solution. *Angewandte Chemie - International Edition*, **2010**, 49, 1967-70	16.4	88
139	Influence of different assignment conditions on the determination of symmetric homodimeric structures with ARIA. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 569-85	4.2	29
138	Shelling the Voronoi interface of protein-protein complexes reveals patterns of residue conservation, dynamics, and composition. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 677-92	4.2	39
137	ATP conformations and ion binding modes in the active site of anthrax edema factor: a computational analysis. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 971-83	4.2	10
136	CASD-NMR: critical assessment of automated structure determination by NMR. *Nature Methods*, **2009**, 6, 625-6	21.6	51
135	Toward a unified representation of protein structural dynamics in solution. *Journal of the American Chemical Society*, **2009**, 131, 16968-75	16.4	98
134	Insights into the enzymatic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei using structural data and molecular dynamics simulation. *Journal of Molecular Biology*, **2009**, 388, 1009-21	6.5	12
133	Accurate NMR structures through minimization of an extended hybrid energy. *Structure*, **2008**, 16, 1305-12	5.2	43
132	Comparative analysis of structural and dynamic properties of the loaded and unloaded hemophore HasA: functional implications. *Journal of Molecular Biology*, **2008**, 376, 517-25	6.5	47

131	3D structure determination of the Crh protein from highly ambiguous solid-state NMR restraints. *Journal of the American Chemical Society*, **2008**, 130, 3579-89	16.4	128
130	SNARE protein mimicry by an intracellular bacterium. *PLoS Pathogens*, **2008**, 4, e1000022	7.6	124
129	Structural biology by NMR: structure, dynamics, and interactions. *PLoS Computational Biology*, **2008**, 4, e1000168	5	94
128	ISD: a software package for Bayesian NMR structure calculation. *Bioinformatics*, **2008**, 24, 1104-5	7.2	28
127	A unifying probabilistic framework for analyzing residual dipolar couplings. *Journal of Biomolecular NMR*, **2008**, 40, 135-44	3	16
126	A structure refinement protocol combining NMR residual dipolar couplings and small angle scattering restraints. *Journal of Biomolecular NMR*, **2008**, 41, 199-208	3	52
125	Graphical analysis of NMR structural quality and interactive contact map of NOE assignments in ARIA. *BMC Structural Biology*, **2008**, 8, 30	2.7	4
124	Probabilistic structure calculation. *Comptes Rendus Chimie*, **2008**, 11, 356-369	2.7	3
123	Structural Bioinformatics and NMR Structure Determination. *Nucleic Acids and Molecular Biology*, **2008**, 123-137		1
122	ARIA2: automated NOE assignment and data integration in NMR structure calculation. *Bioinformatics*, **2007**, 23, 381-2	7.2	404
121	Biskit--a software platform for structural bioinformatics. *Bioinformatics*, **2007**, 23, 769-70	7.2	51
120	Three dimensional structure and implications for the catalytic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei. *Journal of Molecular Biology*, **2007**, 366, 868-81	6.5	18
119	Flexibility and conformational entropy in protein-protein binding. *Structure*, **2006**, 14, 683-93	5.2	113
118	Weighting of experimental evidence in macromolecular structure determination. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 1756-61	11.5	66
117	Clinical and mutational investigations of tyrosinemia type II in Northern Tunisia: identification and structural characterization of two novel TAT mutations. *Molecular Genetics and Metabolism*, **2006**, 88, 184-91	3.7	18
116	NMR in the SPINE Structural Proteomics project. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1150-61		10
115	Error distribution derived NOE distance restraints. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 652-64	4.2	11
114	Determination of dihedral Psi angles in large proteins by combining NH(N)/C(alpha)H(alpha) dipole/dipole cross-correlation and chemical shifts. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 931-9	4.2	4

113	Comparison of different torsion angle approaches for NMR structure determination. *Journal of Biomolecular NMR*, **2006**, 34, 153-66	3	6
112	Functional analysis of early secreted antigenic target-6, the dominant T-cell antigen of Mycobacterium tuberculosis, reveals key residues involved in secretion, complex formation, virulence, and immunogenicity. *Journal of Biological Chemistry*, **2005**, 280, 33953-9	5.4	117
111	Modeling errors in NOE data with a log-normal distribution improves the quality of NMR structures. *Journal of the American Chemical Society*, **2005**, 127, 16026-7	16.4	34
110	Normal mode analysis suggests a quaternary twist model for the nicotinic receptor gating mechanism. *Biophysical Journal*, **2005**, 88, 3954-65	2.9	165
109	The impact of protein flexibility on protein-protein docking. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 126-33	4.2	35
108	Quantitative study of the effects of chemical shift tolerances and rates of SA cooling on structure calculation from automatically assigned NOE data. *Journal of Magnetic Resonance*, **2005**, 175, 92-102	3	30
107	Bayesian estimation of Karplus parameters and torsion angles from three-bond scalar couplings constants. *Journal of Magnetic Resonance*, **2005**, 177, 160-5	3	21
106	SOLARIA: a protocol for automated cross-peak assignment and structure calculation for solid-state magic-angle spinning NMR spectroscopy. *Angewandte Chemie - International Edition*, **2005**, 44, 6151-4	16.4	27
105	SOLARIA: A Protocol for Automated Cross-Peak Assignment and Structure Calculation for Solid-State Magic-Angle Spinning NMR Spectroscopy. *Angewandte Chemie*, **2005**, 117, 6307-6310	3.6	6
104	Influence of chemical shift tolerances on NMR structure calculations using ARIA protocols for assigning NOE data. *Journal of Biomolecular NMR*, **2005**, 31, 21-34	3	8
103	RECOORD: a recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 662-72	4.2	285
102	Inferential structure determination. *Science*, **2005**, 309, 303-6	33.3	268
101	Replica-exchange Monte Carlo scheme for bayesian data analysis. *Physical Review Letters*, **2005**, 94, 018105	7.4	56
100	Bayesian inference applied to macromolecular structure determination. *Physical Review E*, **2005**, 72, 031912	2.4	27
99	Conservation of the biochemical properties of IncA from Chlamydia trachomatis and Chlamydia caviae: oligomerization of IncA mediates interaction between facing membranes. *Journal of Biological Chemistry*, **2004**, 279, 46896-906	5.4	73
98	Complementarity of structure ensembles in protein-protein binding. *Structure*, **2004**, 12, 2125-36	5.2	160
97	Correction of spin diffusion during iterative automated NOE assignment. *Journal of Magnetic Resonance*, **2004**, 167, 334-42	3	51
96	Solution structure of the 30 kDa polysulfide-sulfur transferase homodimer from Wolinella succinogenes. *Biochemistry*, **2004**, 43, 1418-24	3.2	23

95	NOE assignment with ARIA 2.0: the nuts and bolts. *Methods in Molecular Biology*, **2004**, 278, 379-402	1.4	50
94	Refinement of protein structures in explicit solvent. *Proteins: Structure, Function and Bioinformatics*, **2003**, 50, 496-506	4.2	521
93	ARIA: automated NOE assignment and NMR structure calculation. *Bioinformatics*, **2003**, 19, 315-6	7.2	397
92	Structure of the histone mRNA hairpin required for cell cycle regulation of histone gene expression. *Rna*, **2002**, 8, 29-46	5.8	34
91	Pathways and intermediates in forced unfolding of spectrin repeats. *Structure*, **2002**, 10, 1085-96	5.2	71
90	Protein folding in mode space: a collective coordinate approach to structure prediction. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 365-77	4.2	2
89	Solution structure of the coiled-coil trimerization domain from lung surfactant protein D. *Journal of Biomolecular NMR*, **2002**, 24, 89-102	3	9
88	Calculation of Symmetric Oligomer Structures from NMR Data **2002**, 131-161		3
87	Re-face stereospecificity of methylenetetrahydromethanopterin and methylenetetrahydrofolate dehydrogenases is predetermined by intrinsic properties of the substrate. *ChemBioChem*, **2001**, 2, 530-41	3.8	22
86	NMR studies of the sporulation protein SpoIIAA: implications for the regulation of the transcription factor sigmaF in Bacillus subtilis. *Journal of Biomolecular NMR*, **2001**, 19, 293-304	3	8
85	Continuum solvent molecular dynamics study of flexibility in interleukin-8. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 136-45	2.8	24
84	Automated assignment of ambiguous nuclear overhauser effects with ARIA. *Methods in Enzymology* , **2001**, 339, 71-90	1.7	300
83	Structural and functional studies of titin's fn3 modules reveal conserved surface patterns and binding to myosin S1--a possible role in the Frank-Starling mechanism of the heart. *Journal of Molecular Biology*, **2001**, 313, 431-47	6.5	82
82	Re-Face Stereospecificity of Methylenetetrahydromethanopterin and Methylenetetrahydrofolate Dehydrogenases is Predetermined by Intrinsic Properties of the Substrate **2001**, 2, 530		1
81	Efficient sampling in collective coordinate space. *Proteins: Structure, Function and Bioinformatics*, **2000**, 39, 82-8	4.2	29
80	Structure of a PH domain from the C. elegans muscle protein UNC-89 suggests a novel function. *Structure*, **2000**, 8, 1079-87	5.2	25
79	Unraveling the symmetry ambiguity in a hexamer: calculation of the R6 human insulin structure. *Journal of Biomolecular NMR*, **2000**, 16, 93-108	3	32
78	Refinement of the protein backbone angle psi in NMR structure calculations. *Journal of Biomolecular NMR*, **2000**, 16, 47-58	3	25

77	A new approach for applying residual dipolar couplings as restraints in structure elucidation. *Journal of Biomolecular NMR*, **2000**, 16, 245-52	3	83
76	1H, 15N, and 13C resonance assignment of the PH domain from C. elegans UNC-89. *Journal of Biomolecular NMR*, **1999**, 15, 269-70	3	6
75	The structure in solution of the b domain of protein disulfide isomerase. *Journal of Biomolecular NMR*, **1999**, 13, 357-68	3	60
74	StarDOM: from STAR format to XML. *Journal of Biomolecular NMR*, **1999**, 15, 169-72	3	1
73	Influence of non-bonded parameters on the quality of NMR structures: a new force field for NMR structure calculation. *Journal of Biomolecular NMR*, **1999**, 13, 51-9	3	231
72	Contributory presentations/posters. *Journal of Biosciences*, **1999**, 24, 33-198	2.3	
71	The PH superfold: a structural scaffold for multiple functions. *Trends in Biochemical Sciences*, **1999**, 24, 441-5	10.3	159
70	The three-dimensional structure of the HRDC domain and implications for the Werner and Bloom syndrome proteins. *Structure*, **1999**, 7, 1557-66	5.2	110
69	Molecular dynamics and accuracy of NMR structures: Effects of error bounds and data removal. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 453-463	4.2	20
68	Exploring protein interiors: the role of a buried histidine in the KH module fold. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 484-96	4.2	12
67	Classification of protein sequences by homology modeling and quantitative analysis of electrostatic similarity. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 379-87	4.2	76
66	Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory. *Journal of Molecular Biology*, **1999**, 285, 727-40	6.5	33
65	Functionally important correlated motions in the single-stranded DNA-binding protein encoded by filamentous phage Pf3. *Journal of Molecular Biology*, **1999**, 287, 569-77	6.5	18
64	Ambiguous NOEs and automated NOE assignment. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **1998**, 32, 107-139	10.4	185
63	The three-dimensional structure of a type I module from titin: a prototype of intracellular fibronectin type III domains. *Structure*, **1998**, 6, 1291-302	5.2	39
62	Essential spaces defined by NMR structure ensembles and molecular dynamics simulation show significant overlap. *Proteins: Structure, Function and Bioinformatics*, **1998**, 31, 370-382	4.2	58
61	Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 905-21		14106
60	Heteronuclear relaxation study of the PH domain of beta-spectrin: restriction of loop motions upon binding inositol trisphosphate. *Journal of Molecular Biology*, **1998**, 280, 879-96	6.5	33

59	Are there non-trivial dynamic cross-correlations in proteins?. *Journal of Molecular Biology*, **1998**, 279, 911-20	6.5	45
58	Refined structure, DNA binding studies, and dynamics of the bacteriophage Pf3 encoded single-stranded DNA binding protein. *Biochemistry*, **1997**, 36, 9120-35	3.2	25
57	Automated NOESY interpretation with ambiguous distance restraints: the refined NMR solution structure of the pleckstrin homology domain from beta-spectrin. *Journal of Molecular Biology*, **1997** , 269, 408-22	6.5	395
56	Solution structure of the spectrin repeat: a left-handed antiparallel triple-helical coiled-coil. *Journal of Molecular Biology*, **1997**, 273, 740-51	6.5	135
55	The structure of a novel insecticidal neurotoxin, omega-atracotoxin-HV1, from the venom of an Australian funnel web spider. *Nature Structural Biology*, **1997**, 4, 559-66		149
54	The solution structure of the first KH domain of FMR1, the protein responsible for the fragile X syndrome. *Nature Structural Biology*, **1997**, 4, 712-6		71
53	Solution structure of the DNA-binding domain and model for the complex of multifunctional hexameric arginine repressor with DNA. *Nature Structural Biology*, **1997**, 4, 819-26		104
52	The folding catalyst protein disulfide isomerase is constructed of active and inactive thioredoxin modules. *Current Biology*, **1997**, 7, 239-45	6.3	185
51	Functional diversity of PH domains: an exhaustive modelling study. *Folding & Design*, **1997**, 2, 343-55		30
50	Tertiary structure prediction using mean-force potentials and internal energy functions: successful prediction for coiled-coil geometries. *Folding & Design*, **1997**, 2, S47-52		17
49	Ambiguous distance data in the calculation of NMR structures. *Folding & Design*, **1997**, 2, S53-7		49
48	1H and 15N NMR resonance assignments and secondary structure of titin type I domains. *Journal of Biomolecular NMR*, **1997**, 9, 2-10	3	8
47	Floating stereospecific assignment revisited: application to an 18 kDa protein and comparison with J-coupling data. *Journal of Biomolecular NMR*, **1997**, 9, 245-58	3	100
46	Structure determination of the N-terminal thioredoxin-like domain of protein disulfide isomerase using multidimensional heteronuclear 13C/15N NMR spectroscopy. *Biochemistry*, **1996**, 35, 7684-91	3.2	172
45	Three-dimensional structure and stability of the KH domain: molecular insights into the fragile X syndrome. *Cell*, **1996**, 85, 237-45	56.2	258
44	Structure calculation from NMR data. *Current Opinion in Structural Biology*, **1996**, 6, 617-23	8.1	41
43	High resolution NMR solution structure of the leucine zipper domain of the c-Jun homodimer. *Journal of Biological Chemistry*, **1996**, 271, 13663-7	5.4	85
42	Molecular replacement with NMR models using distance-derived pseudo B factors. *Acta Crystallographica Section D: Biological Crystallography*, **1996**, 52, 973-82		14

41	Calculation of symmetric multimer structures from NMR data using a priori knowledge of the monomer structure, co-monomer restraints, and interface mapping: The case of leucine zippers. *Journal of Biomolecular NMR*, **1996**, 8, 193-206	3	34
40	Internal repeats in the BRCA2 protein sequence. *Nature Genetics*, **1996**, 13, 22-3	36.3	173
39	Three-dimensional structure of the single-stranded DNA-binding protein encoded by gene V of the filamentous bacteriophage M13 and a model of its complex with single-stranded DNA. *FEMS Microbiology Reviews*, **1995**, 17, 57-72	15.1	4
38	Calculation of protein structures with ambiguous distance restraints. Automated assignment of ambiguous NOE crosspeaks and disulphide connectivities. *Journal of Molecular Biology*, **1995**, 245, 645-60	6.5	324
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